

Bose-Einstein condensates in multiple well potentials from a variational path integral

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We apply a path integral variational approach to obtain analytical expressions for condensate wave functions of an ultracold, interacting trapped Bose gases. As in many recent experiments, the particles are confined in a 1D or 3D harmonic oscillator trap which is superimposed by a periodic potential in one direction. Based on the first order cumulant expansion with respect to a harmonic trial action, and employing a mean-field approximation, optimal variational parameters are obtained by minimizing an analytical expression for the ground state energy. Our largely analytical results for energy and condensate wave function are in good agreement with fully numerical calculations based on the Gross-Pitaevskii equation.

I. INTRODUCTION

Ultracold atomic gases trapped in harmonic and periodic potentials are in the focus of current theoretical and experimental research¹⁻⁴. The number of energetically available potential wells can be tuned through the strength of the confining trap, and the parameters of the standing wave light field.

In fact, there are very many investigations for the extreme case of effectively just two potential wells⁵⁻¹⁵, developing Josephson oscillations for an appropriate choice of parameters. On the other hand, investigations in the limit of (almost) periodic potentials can rely on Bloch theory. In that case one is often able to choose a description in terms of the lowest band only^{16,17}.

The influence of atomic interactions in current experiments can be observed through self-trapping both in double well systems⁵, and in potentials with many potential wells^{17,18}. More recently, Trotzky *et al.*¹⁹ studied relaxation dynamics in an interacting bosonic many-body system in an optical lattice combined with a shallow harmonic trap, such that about forty potential wells are of relevance for the dynamics. Since the number of particles per site is very small, full quantum calculations involving the N-particle state can be carried out on the basis of the celebrated Bose-Hubbard model¹⁻⁴.

In this work we are interested in the limit of many particles per well and a mean-field description of the ultracold Bose gas in terms of a single condensate wave function $\phi_0(\mathbf{r})$ ²⁰⁻²². Instead of a direct numerical determination of the wave function as the ground state solution of the Gross-Pitaevskii equation, however, we aim at a largely analytical approach with a path integral description as our starting point.

Path integrals have proven indispensable in many areas of physics, ranging from quantum mechanics and quantum field theory to important applications in both quantum and classical statistical physics²³⁻²⁵. In connection to cold atomic gases, a path integral approach for the quantum field dynamics helps to derive Gross-Pitaevskii-type stochastic equations that contain damping and thermal fluctuations²⁶ (see also²⁷). More recently, we investigated the Bose-Einstein condensate wave function in a

double-well potential within the Feynman path integral variational approach²⁸. In the present paper we expand our earlier work to a trapped condensate with an additional periodic potential in one dimension. Remarkably, our method leads to the same variational energy as obtained from a simple Gaussian ansatz for the wave function. However, the Feynman path integral variational approach allows to obtain a much improved expression for the condensate wave function as shown in this work.

II. THE FEYNMAN PATH INTEGRAL

We examine N Bosons with repulsive interaction confined in a three dimensional harmonic trap, which is superposed with a periodic potential in x direction. Such a setup is realized in many current experiments^{3,4,16,18,19}. The N-body potential thus reads

$$V = \frac{1}{2} \sum_{i=1}^N (\Omega_x^2 x_i^2 + \Omega_y^2 y_i^2 + \Omega_z^2 z_i^2) + \frac{A}{2} \sum_{i=1}^N (\cos(2kx_i) + 1) + g \sum_{i<j}^N \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (1)$$

where Ω_x, Ω_y , and Ω_z are harmonic oscillator frequencies of the trap, A is proportional to the intensity of a standing wave laser beam and k the corresponding wave number. The interatomic interaction is taken care of by an effective delta-shaped pseudopotential where g is proportional to the s-wave scattering length $a > 0$. We exploit a harmonic trial Lagrangian

$$L_0 = \frac{1}{2} \sum_{i=1}^N (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) - \frac{1}{2} \sum_{i=1}^N (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2), \quad (2)$$

for which the propagator is known in closed form, and as a path integral may be written as

$$P_0 = \int_{x_i,0}^{x_f,t} D^N[x(\tau)] \exp(iS_0) \quad (3)$$

with $S_0 = \int d\tau L_0$. Later, $\omega_x, \omega_y, \omega_z$ are considered to be variational parameters. In the following, we calculate the

propagator for the N -body case with potential V from (1). Since

$$P = \langle x_f | \exp(-iHt) | x_i \rangle = \sum_{n=0}^{\infty} \exp(-iE_n t) \phi_n(x_f) \phi_n^*(x_i), \quad (4)$$

and replacing $t \rightarrow -i\tau$, we find the ground state energy and the condensate wave function in the limit $\tau \rightarrow \infty$. With the harmonic oscillator as a trial system, we can express the propagator of the entire system as

$$P = \int_{x(0)}^{x(t)} D^N[x(\tau)] \exp(iS) = P_0 \langle \exp[i(S - S_0)] \rangle_{S_0}. \quad (5)$$

The bracket $\langle \dots \rangle_{S_0} = \int D^N[x] \exp[iS_0](\dots) / P_0$ denotes the “average” with respect to the trial “probability” density functional $\exp(iS_0)$. Similar to related expansions in probability theory, and following Bachmann et al.²⁹, this propagator can be expanded in terms of cumulants. In first order we get from equ. (5)

$$P \approx P_0 \exp[i \langle S - S_0 \rangle_{S_0}]. \quad (6)$$

Similar to standard probability theory it is possible to obtain mean values from generating functionals²³

$$\Phi[f(t)] = \left\langle \exp \left[i \int_0^t f(\tau) x(\tau) d\tau \right] \right\rangle_{S_0}. \quad (7)$$

Average values of $x(\tau)$, for instance are obtained from

$$\langle x(\tau) \rangle_{S_0} = -i \frac{\delta \Phi[f(\tau)]}{\delta f(\tau)} \Big|_{f=0} \quad (8)$$

and

$$\langle x(\tau)^2 \rangle_{S_0} = (-i)^2 \frac{\delta^2 \Phi[f(\tau)]}{\delta f(\tau)^2} \Big|_{f=0}. \quad (9)$$

The generating functional can be expressed in terms of the difference between the action of a driven harmonic oscillator S'_0 and the action of a usual harmonic oscillator S_0

$$\Phi[f(t)] = \langle \exp[i(S'_0 - S_0)] \rangle_{S_0} = \exp[i(S'_{cl} - S_{cl})]. \quad (10)$$

Here $S'_0 = S_0 + \int f(\tau) x(\tau) d\tau$ represents the action of a driven oscillator with external force $f(\tau)$. For harmonic systems the path integral can be evaluated in closed form. One finds $P \sim \exp(iS_{cl})$ for the propagator with the action $S_{cl} = S_0[x_{cl}]$ along the classical path. Thus,

$$\langle x(\tau) \rangle_{S_0} = \frac{\delta S'_{cl}}{\delta f(\tau)} \Big|_{f=0} \quad (11)$$

and

$$\langle x(\tau)^2 \rangle_{S_0} = \left[-i \frac{\delta^2 S'_{cl}}{\delta f(\tau)^2} + \left(\frac{\delta S'_{cl}}{\delta f(\tau)} \right)^2 \right] \Big|_{f=0}. \quad (12)$$

The analytical expression in one dimension, for simplicity, reads²³

$$S'_{cl} = \frac{\omega_x}{2 \sin(\omega_x t)} \left(((x_i^2 + x_f^2) \cos(\omega t) - 2x_i x_f) + \frac{2x_f}{\omega_x} \int_0^t d\tau f(\tau) \sin \omega_x \tau + \frac{2x_i}{\omega_x} \int_0^t d\tau f(\tau) \sin \omega_x(t - \tau) - \frac{2}{\omega_x^2} \int_0^t d\tau \int_0^\tau ds f(s) f(\tau) \sin \omega_x \tau \sin \omega_x(t - \tau) \right) \quad (13)$$

and leads us directly to the Green function

$$g(t, \tau) = \langle x^2 \rangle_{S_0} - \langle x \rangle_{S_0}^2 = \frac{i}{\omega_x} \frac{\sin \omega_x(t - \tau) \sin \omega_x \tau}{\sin \omega_x t}. \quad (14)$$

Moreover, we have to calculate averages of more complicated functions of $x(\tau)$. These can be obtained along similar lines from the generating functional. The contribution of the cosine potential, for instance, is

$$\langle \cos(2kx) \rangle_{S_0} = \exp[-2k^2 g(t, \tau)] \cos(2k \langle x \rangle_{S_0}). \quad (15)$$

For the interatomic interaction, we use the Fourier representation

$$\delta(x_i - x_j) = \frac{1}{2\pi} \int dq \exp[iq(x_i - x_j)]. \quad (16)$$

Taking the Gaussian average, we find

$$\langle \exp[iq(x_i - x_j)] \rangle_{S_0} = \exp \left[-q^2 \left(g(t, \tau) + \langle x_i \rangle_{S_0} \langle x_j \rangle_{S_0} - \langle x_i x_j \rangle_{S_0} \right) \right]. \quad (17)$$

Using the mean field factorization $\langle x_i x_j \rangle_{S_0} = \langle x_i \rangle_{S_0} \langle x_j \rangle_{S_0}$, we obtain

$$\langle \delta(x_i(\tau) - x_j(\tau)) \rangle_{S_0} = \sqrt{\frac{1}{4\pi g(t, \tau)}}. \quad (18)$$

Ground state properties (ground state energy and condensate wave function) can be obtained by taking the limit $t \rightarrow -i\infty$ of the full expression of the propagator in Eq. (6). In our case, the result for the energy is

$$E_0(\omega_x, \omega_y, \omega_z)/N = \frac{\omega_x}{4} + \frac{\omega_y}{4} + \frac{\omega_z}{4} + \frac{\Omega_x^2}{4\omega_x} + \frac{\Omega_y^2}{4\omega_y} + \frac{\Omega_z^2}{4\omega_z} + \frac{A}{2} + \frac{A}{2} \exp\left(-\frac{k^2}{\omega_x}\right) + \frac{g(N-1)}{2} \left(\frac{1}{2\pi}\right)^{3/2} \sqrt{\omega_x \omega_y \omega_z}. \quad (19)$$

Remarkably, this expression can also be obtained from a more direct variational approach with Gaussian trial wave functions with variances $1/2w_x$, $1/2w_y$ and $1/2w_z$ for the respective directions.

Our variational condensate wave function can be read off in the limit $t \rightarrow -i\infty$ and we obtain

$$\phi_0(x, y, z) \sim \exp \left[- \left(\frac{\Omega_x^2}{4\omega_x} + \frac{\omega_x}{4} \right) x^2 - \left(\frac{\Omega_y^2}{4\omega_y} + \frac{\omega_y}{4} \right) y^2 - \left(\frac{\Omega_z^2}{4\omega_z} + \frac{\omega_z}{4} \right) z^2 - \frac{A}{2} \lambda_0(x) \right] \quad (20)$$

with

$$\lambda_0(x) = -\frac{1}{\omega_x} (\gamma - \text{Ci}(2kx) + \ln(2kx)) + \frac{1}{2} \sum_{j=1}^{\infty} \frac{2^{2j+1} \omega_x^{j-1} e^{-\frac{k^2}{\omega_x}}}{(2j)^2} x^{2j} \theta(j), \quad (21)$$

$$\theta(j) = \frac{\Gamma(j+1) - \Gamma\left(j+1, -\frac{k^2}{\omega_x}\right)}{\Gamma(2j)}. \quad (22)$$

Here $\gamma \simeq 0.577216$ is Euler's constant, $\text{Ci}(x)$ is the cosine integral function, $\Gamma(x)$ is the Euler gamma function and $\Gamma(x, y)$ is the incomplete Euler gamma function. We can normalize this wave function by using the condition $\int |\phi_0(\mathbf{r})|^2 d^3\mathbf{r} = 1$. The condensate wave function decomposes in a product of functions for each dimension. In y - and z -dimension it turns out to be Gaussian, as could be expected because the condensate is harmonically trapped in these directions. However, in x -direction due to the additional periodic potential, a contribution $A\lambda_0(x)/2$ in the exponential modifies the Gaussian shape significantly. A damped periodic modulation of the condensate wave function along x is obtained. We numerically minimize the energy functional with respect to the variational parameters and obtain the optimal ω_x , ω_y and ω_z , which are then used to compute the condensate wave function $\phi_0(\mathbf{r})$.

III. COMPARISON WITH FULL NUMERICS

Next we compare the quality of our results from the Feynman path integral variational approach with a numerical mean-field calculation obtained through imaginary-time propagation of the Gross-Pitaevskii equation. The comparison is done with 1D and 3D isotropic, and 3D anisotropic harmonic traps. Using the Feynman path integral approach in one dimension, we get the ground state energy of the entire system

$$\frac{E_0(\omega_x)}{N} = \frac{\omega_x}{4} + \frac{\Omega_x^2}{4\omega_x} + \frac{A}{2} + \frac{A}{2} \exp\left(-\frac{k^2}{\omega_x}\right) + \frac{g(N-1)}{2} \sqrt{\frac{\omega_x}{2\pi}}. \quad (23)$$

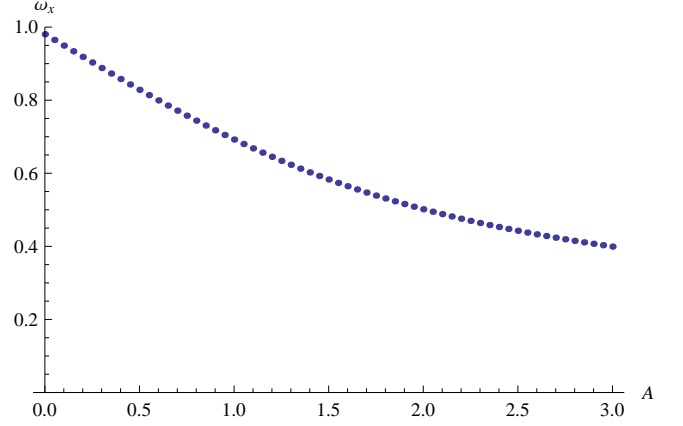


FIG. 1. Minimizing parameter ω_x for the 1D system as a function of A for $k = 0.744$, $\Omega_x = 1$, $gN = 0.1$.

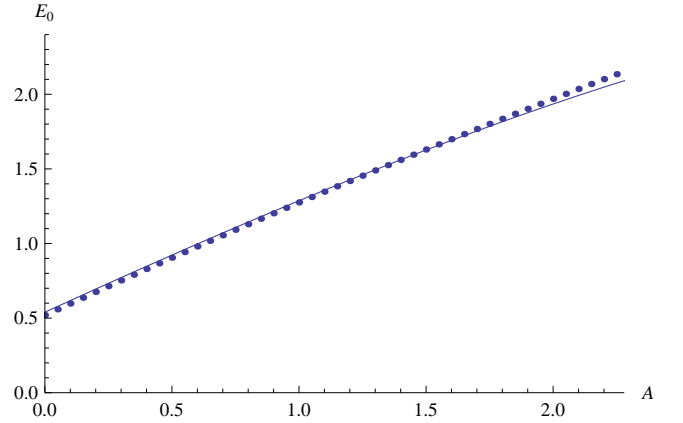


FIG. 2. Ground state energy as a function of A for the 1D system. The solid line is the numerical solution of the Gross-Pitaevskii equation and the dots are obtained from path integral theory for $k = 0.744$, $\Omega_x = 1$, $gN = 0.1$.

The corresponding condensate wave function is

$$\phi_0(x) \sim \exp \left[- \left(\frac{\Omega_x^2}{4\omega_x} + \frac{\omega_x}{4} \right) x^2 + \frac{A}{2} \lambda_0(x) \right]. \quad (24)$$

We minimize this energy by solving $\partial E_0(\omega_x)/\partial \omega_x = 0$ for a small repulsive self interaction $g(N-1) \approx gN = 0.1$. The relation between the minimizing parameter ω_x and A is shown in Fig. 1. The comparison between variational energy and numerically exact Gross-Pitaevskii energy is displayed in Fig. 2. We next insert these optimal values for ω_x into Eq. (24) and normalize. In Fig. 3 we compare this variational wave function (24) with the numerically exact solution of the Gross-Pitaevskii equation for various parameters. The corresponding potentials range from almost double-well type (for strong trapping confinement, $\Omega = 1$) to genuine multiple-well shape for weaker traps ($\Omega = 0.1, 0.02$). In the first case, the condensate wave function Eq. (24) is separated into two

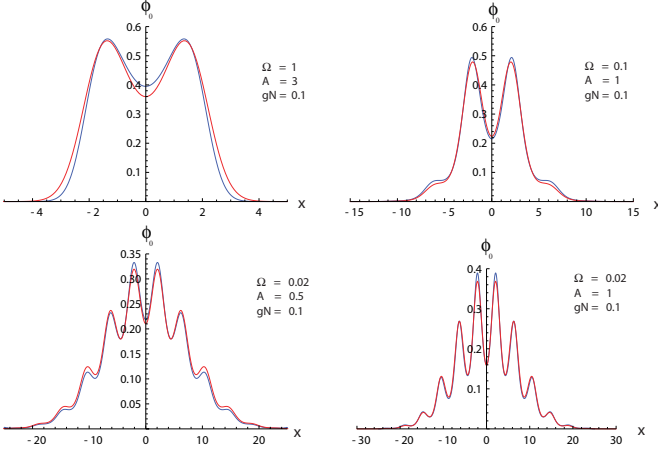


FIG. 3. Condensate wave function $\phi_0(x)$ for the one dimensional system. The red lines are the results of imaginary time propagation of the Gross-Pitaevskii equation, the blue lines are calculated by our variational path integral approach.

peaks which are symmetrically centered around the origin. In the latter cases, the condensate wave function reflects the multiple-well structure of the confining potential (see Fig. 3).

We observe that over a wide range of potential parameters, the condensate wave function from the path integral variational approach agrees very well with the numerical solution of the Gross-Pitaevskii equation.

Equivalently, Bose-Einstein condensate wave functions in 3D can be determined by minimizing the ground state energy in equ. (19), see Fig. 4 for the choices $\Omega = \Omega_x = \Omega_y = \Omega_z = 1$ and $gN = 1$. We obtain the values of the minimizing parameters and from these the value of the ground state energy. Inserting these optimal $\omega_x, \omega_y, \omega_z$ into equ. (20) and normalizing the wave function, we obtain ϕ_0 . Cuts of the densities $n_0 = \phi_0^2$ at $z = 0$ are shown in Fig. 5 at $gN = 1$ for various trap parameters: top: $\Omega = 1, A = 3$, double-well type; middle and bottom: $\Omega = 0.02$ multiple-well type, with $A = 0.5$ (middle) and $A = 1.0$ (bottom). Again we observe remarkable agreement with numerically exact solutions of the Gross-Pitaevskii equation. Finally, in Fig. 6 we exhibit results for anisotropic confining traps (interaction parameter $gN = 1$). The first graphs correspond to a pan cake type condensate in x -direction ($\Omega_x = 1, \Omega_y = \Omega_z = 0.05$) with a fairly strong cosine potential $A = 3$, which leads to a very narrow and double-well-like confinement in x direction (Fig. 6, top). As a second example (Fig. 6, middle) we present plots for a cigar type confinement in x -direction, ($\Omega_x = 0.02, \Omega_y = \Omega_z = 1$) and barrier height $A = 1$. Thirdly, there is a slightly anisotropic and weakly confining example with $\Omega_x = 0.02, \Omega_y = \Omega_z = 0.01$. In this case the barrier height is $A = 1$ so that many potential wells are populated. As before, the ground state energies of these three examples and the minimizing parameters can be determined from equ. (20) with results shown in

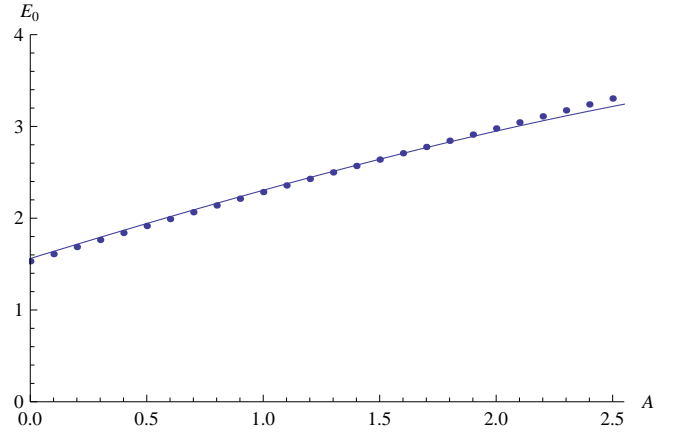


FIG. 4. Ground state energy in 3D as a function of A . The solid line is calculated from the Gross-Pitaevskii equation and the dots are calculated by path integral variational theory for $k = 0.744, \Omega_x = \Omega_y = \Omega_z = 1, gN = 1$.

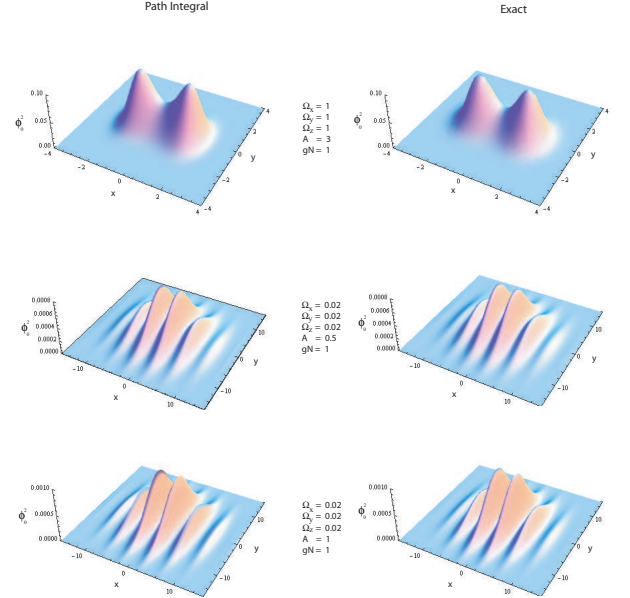


FIG. 5. Density cuts of the variational condensate wave functions at $z = 0$ in 3D (left column) compared with numerically exact solutions of the Gross-Pitaevskii equation for an isotropic confining trap (right column).

Table 1.

IV. CONCLUSION

We have studied Bose-Einstein condensates in a multiple-well potential applying Feynman path integral variational theory. As in recent experiments, the trap consists of a harmonic confinement superimposed by a periodic (cosine) standing wave field. The calculations

A	Ω_x	Ω_y	Ω_z	ω_x	ω_y	ω_z	E_0	$E_{0,GP}$
3	1	0.05	0.05	0.4019	0.0490	0.0490	2.652	2.463
1	0.02	1	1	0.01640	0.9960	0.9960	1.514	1.415
1	0.02	0.01	0.01	0.01995	0.00996	0.00996	0.520	0.414

TABLE I. Optimizing variational parameters ω_x , ω_y and ω_z for the three examples for 3D anisotropic traps. The corresponding ground state energies from path integral theory E_0 and from Gross-Pitaevskii numerics $E_{0,GP}$ are in fair agreement.

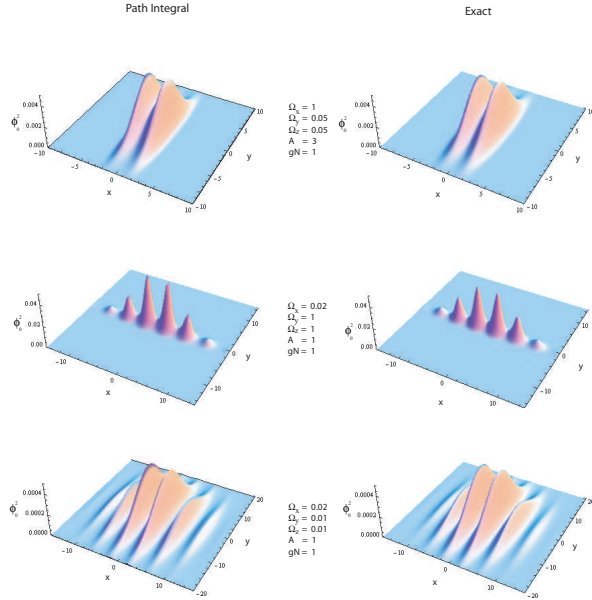


FIG. 6. Density cuts of the condensates at $z = 0$ in 3D compared with the exact solutions of the Gross-Pitaevskii equation for anisotropic traps.

are carried out within the first cumulant approximation measured with respect to a harmonic trial action. The advantage of this method is that we obtain analytical expressions for ground state energy and condensate wave function. These results are in remarkable agreement with fully numerical calculations based on the Gross-Pitaevskii equation. We concentrate on a fairly weak interaction parameter gN , no larger than unity. For stronger interactions deviations from Gross-Pitaevskii theory begin to appear. It is very remarkable that our Feynman path integral variational approach leads to the same ground state energy as a purely Gaussian trial wave function. However, the path integral approach offers a highly non-trivial expression for the condensate wave function with strongly non-Gaussian shape. In fact, we find very good agreement with the exact condensate wave function as obtained from a numerical solution of the Gross-Pitaevskii equation.

In future investigations we aim to drop the factorization approximation $\langle x_i x_j \rangle \approx \langle x_i \rangle \langle x_j \rangle$, such as to be able to go beyond mean-field Gross-Pitaevskii theory.

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